

# Soliton Automata\*

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Soliton valves have been proposed as molecular switching elements. We introduce a mathematical model of the logics aspects of soliton switching called soliton automaton. We prove a characterization of strongly deterministic soliton automata, certain important properties of their transition monoids, and a characterization of the class of automata which can be simulated by soliton automata. Finally the cost of this simulation is discussed. © 1990 Academic Press, Inc.

## 1. INTRODUCTION

There are various speculations about the direction of the development of future computer architecture. In this paper we provide a mathematical model and several mathematical results which could be used to determine the computational power of one type of a proposed switching device, the “soliton valve” (see [2–4]).

Research in bioelectronics has proposed several chemical structures as basic building blocks for future computers. For a survey see [3] and the proceedings volume [5]. Among these, “soliton valves” seem to be very interesting candidates. Their switching behaviour is based on the effects on a soliton wave travelling along a molecule chain. The main example discussed in the literature works with polyacetylene chains as shown in Fig. 1. Ignoring the physico-chemical details, the effect of a soliton wave propagating along such a chain is to exchange all single and double bonds. In terms of switching logic this amounts to the action of a flip-flop.

In this paper we are only interested in the logics aspects of “soliton valves.” For the physico-chemical background see [8]. We define “soliton graphs” and “soliton

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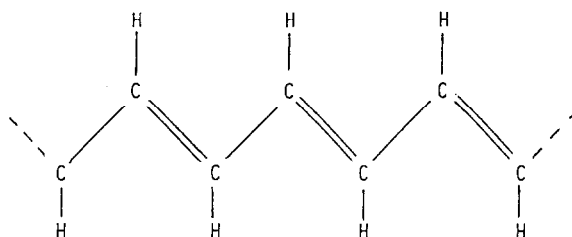


FIG. 1. (CH)-chain.

automata” based on soliton graphs as a mathematical model of “soliton valves.” We then single out “deterministic” and “strongly deterministic” soliton automata. For obvious reasons these are very important cases. From an application point of view the class of deterministic soliton automata is more natural. However, mathematical considerations make us restrict our attention to the subclass of strongly deterministic soliton automata for most of this paper. A characterization of the corresponding graphs is provided. They turn out to be “sums” of either trees or a special kind of soliton graph, called “chestnuts.”

We use the transition monoids of soliton automata as a criterion to determine their computational power. The transition monoids of strongly deterministic soliton automata are shown to be direct products of primitive permutation groups. The class of primitive permutation groups obtained in this way properly contains the class of finite symmetric groups and is itself properly contained in the class of all finite primitive groups. This shows that exactly the group automata can be simulated by soliton automata—though possibly at a tremendous cost. Based on these findings, an assessment of the computational power of products of soliton automata has been obtained in [11].

The paper ends with a tentative evaluation of these results and a brief discussion of a few related open questions.

## 2. BASIC NOTIONS

In this section we review a few basic notions required in the rest of this paper.

An *alphabet* is a finite, non-empty set. Let  $X$  be an alphabet. Then  $X^*$  denotes the set of *words* over  $X$  including the *empty word*  $\varepsilon$ , and  $X^+ = X^* \setminus \{\varepsilon\}$ . With the concatenation as multiplication,  $X^*$  and  $X^+$  are the free monoid and the free semigroup over  $X$ . For a word  $w \in X^*$ ,  $|w|$  is the *length* of  $w$ ; in particular,  $|\varepsilon| = 0$ .

A *deterministic finite automaton* is a construct  $\mathcal{A} = (S, X, \delta)$  with the following properties:  $S$  is a finite, non-empty set, the set of *states*;  $X$  is an alphabet, the *input alphabet*;  $\delta$  is a mapping of  $S \times X$  into  $S$ , the *transition function*. As nearly all automata considered in this paper are deterministic and finite, we just use the term “automaton” to mean “deterministic finite automaton.” Automata without outputs

as defined here are also referred to as *semi-automata* in the literature. Occasionally we also need to consider a *non-deterministic automaton*. In this case, the transitions are defined by a mapping  $\delta$  of  $S \times X$  into  $2^S$  instead of into  $S$ .

Let  $\mathcal{A} = (S, X, \delta)$  be an automaton. As usual,  $\delta$  is extended to a mapping of  $S \times X^*$  into  $S$  by

$$\delta(s, \varepsilon) = s$$

and

$$\delta(s, wx) = \delta(\delta(s, w), x)$$

for  $s \in S$ ,  $w \in X^*$ , and  $x \in X$ . For  $w \in X^*$  let  $\delta_w$  denote the transformation of  $S$  which is given by

$$\delta_w(s) = \delta(s, w)$$

for  $s \in S$ . Let

$$T(\mathcal{A}) = \{ \delta \mid \delta \in S^S \text{ and } \delta = \delta_w \text{ for some } w \in X^* \}.$$

With the usual multiplication of mappings the set  $T(\mathcal{A})$  is a monoid, the *transition monoid* of  $\mathcal{A}$ . Clearly,  $\delta_u \delta_v = \delta_{uv}$  for any  $u, v \in X^*$ . Hence, the mapping  $X^* \rightarrow T(\mathcal{A})$ :  $w \mapsto \delta_w$  is a surjective morphism.

To a certain extent, the transition monoid can be used to describe the structure of an automaton and to compare the structure of automata. Given automata  $\mathcal{A}_1$  and  $\mathcal{A}_2$ , we say that  $\mathcal{A}_1$  (*weakly*) *simulates*  $\mathcal{A}_2$  if  $T(\mathcal{A}_2)$  *divides*  $T(\mathcal{A}_1)$ , that is, if  $T(\mathcal{A}_2)$  is the homomorphic image of a submonoid of  $T(\mathcal{A}_1)$ . In such a case we write  $\mathcal{A}_1 \succcurlyeq \mathcal{A}_2$  and  $T(\mathcal{A}_2) \mid T(\mathcal{A}_1)$ . Observe that with this notion of simulation the automata may not only have different sets of states but also even different input alphabets.

Another type of comparison of automata is achieved by automaton morphisms. For  $i = 1, 2$  let  $\mathcal{A}_i = (S_i, X_i, \delta_i)$  be automata. A morphism of  $\mathcal{A}_1$  into  $\mathcal{A}_2$  is a pair  $\psi = (\psi_S, \psi_X)$  of mappings  $\psi_S: S_1 \rightarrow S_2$  and  $\psi_X: X_1 \rightarrow X_2$  which satisfies the equation

$$\psi_S(\delta_1(s, x)) = \delta_2(\psi_S(s), \psi_X(x))$$

for every  $s \in S_1$  and every  $x \in X_1$ . The morphism  $\psi$  is an automaton isomorphism of  $\mathcal{A}_1$  onto  $\mathcal{A}_2$  if both  $\psi_S$  and  $\psi_X$  are bijective mappings.

For any finite non-empty index set  $I$  and for  $i \in I$  let  $\mathcal{A}_i = (S_i, X_i, \delta_i)$  be an automaton. Their product

$$\prod_{i \in I} \mathcal{A}_i$$

is the automaton  $\mathcal{A} = (S, X, \delta)$ , where  $S$  is the Cartesian product of all  $S_i$ ,  $X$  is the disjoint union of all  $X_i$ , and

$$\delta((s_i)_{i \in I}, x) = (s'_i)_{i \in I},$$

where

$$s'_i = \begin{cases} \delta_i(s_i, x), & \text{if } x \in X_i \\ s_i, & \text{otherwise.} \end{cases}$$

Clearly,  $T(\mathcal{A}) \simeq \prod_{i \in I} T(\mathcal{A}_i)$ , and the isomorphism is induced by the inclusion mapping of the sets  $X_i$  in  $X$ .

### 3. DEFINITION OF THE MODEL

As seems natural from the examples discussed in the Introduction our formal model is based on graph theoretical notions. In order to fix terminology and notation we briefly review the necessary definitions.

A *graph* is a pair  $G = (N, E)$  with  $N$  a set, the set of *nodes*, and with  $E \subseteq N \times N$  the set of *edges*. In this paper we consider finite, non-empty undirected graphs only; therefore, in the sequel we assume without special mentioning that  $N$  is finite and non-empty, and that  $E^{-1} \subseteq E$ , that is, for all nodes  $n, n' \in N$  one has  $(n', n) \in E$  if  $(n, n') \in E$ . However, if  $(n, n') \in E$  then both  $(n, n')$  and  $(n', n)$  represent the same edge of  $G$ . Observe that with this definition any two nodes of a graph can be connected by at most one edge.

Let  $\mathbb{N}_0$  denote the set of non-negative integers. A mapping  $w: N \times N \rightarrow \mathbb{N}_0$  is called a *weight function* if

$$w(n, n') = \begin{cases} 0 & \text{for } (n, n') \notin E; \\ w(n', n) > 0 & \text{for } (n, n') \in E. \end{cases}$$

A triple  $G = (N, E, w)$  with  $(N, E)$  a graph and  $w$  a weight function on  $(N, E)$  is called a *weighted graph*. Clearly, more general types of weight functions could be considered; however, for this paper the notion as introduced is general enough.

For a node  $n \in N$  the set

$$V(n) = \{n' \mid (n, n') \in E\}$$

is the *vicinity* (neighbourhood) of  $n$ , the integer

$$d(n) = |V(n)|$$

is its *degree*, and

$$w(n) = \sum_{n' \in V(n)} w(n, n')$$

is its *weight*. A node  $n$  is said to be *isolated* if  $d(n) = 0$ , *exterior* if  $d(n) = 1$ , and *interior* if  $d(n) > 1$ .

The following definition abstracts from the physico-chemical details of the examples of "soliton valves" built from polyacetylene chains as proposed in [2], for instance. A more general definition is conceivable, but would almost certainly lead too far away from chemical and physical facts as currently available.

**DEFINITION 3.1.** A *soliton graph* is a weighted graph  $G = (N, E, w)$  which satisfies the following conditions:

- (a)  $G$  has no loops; that is  $(n, n) \notin E$  for all  $n \in N$ ;
- (b) every component (that is, maximal connected subgraph) of  $G$  has at least one exterior node;
- (c) for every  $n \in N$  one has  $1 \leq d(n) \leq 3$ ;
- (d) if  $n$  is an exterior node then  $w(n) \in \{1, 2\}$ ;
- (e) for every  $n \in N$  with  $d(n) \in \{2, 3\}$  one has  $w(n) = d(n) + 1$ .

A soliton graph  $G = (N, E, w)$  models the "soliton valves" of [2] as follows: Each interior node  $n$  represents a C atom or a C-H group depending on whether  $d(n)$  is 3 or 2, respectively. An edge  $(n, n')$  of weight  $i \in \{1, 2\}$  represents a (CH)-chain with alternating double and single bonds which connects the C atoms of  $n$  and  $n'$  and which begins and ends with an  $i$ -fold bond. As the length of such chains does not affect the logic of the model we usually draw them as length 1 chains; physico-chemical reasons may require different lengths for actual realizations. Finally, exterior nodes represent the connection to surrounding structures. Certain proposals as to their chemical realization can be found in [2]. Figure 2 shows an example of a soliton graph and a possible chemical interpretation. The weights of edges are indicated by single and double lines.

A simple case of a "conjugated system" in a soliton graph would be a path  $n_0, n_1, \dots, n_k$  such that  $|w(n_i, n_{i+1}) - w(n_{i+1}, n_{i+2})| = 1$  for  $i = 0, 1, \dots, k-2$ . That is,

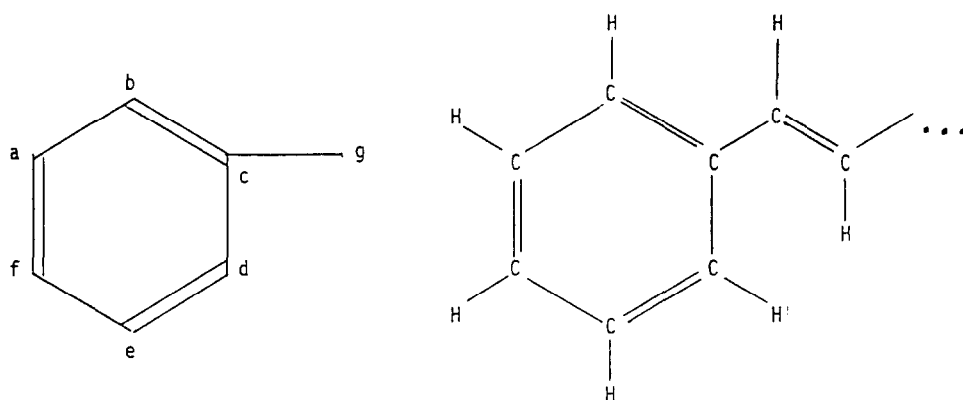


FIG. 2. A soliton graph with one of its interpretations.

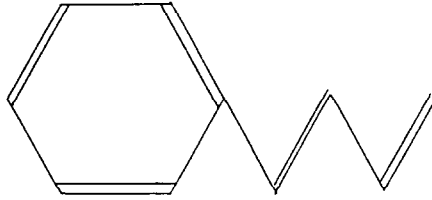


FIG. 3. A soliton graph with an edge traversed several times [2].

such a path would have alternating single and double bonds in the chemical interpretation. A soliton propagating along such a path will exchange single and double bonds. In our model this corresponds to exchanging weights 1 and 2.

However, this is too simple for a correct definition of a model of soliton propagation. Figure 3 shows an example adopted from [2] in which edges would be traversed more than once on a path. Thus using statically conjugated systems as the basis for a definition of the switching behaviour that models soliton movement would be inadequate. The following more complicated definition is required:

**DEFINITION 3.2.** Let  $G = (N, E, w)$  be a soliton graph. A path  $n_0, n_1, \dots, n_k$  of  $G$  is called a *partial soliton path* if the following conditions hold:

- (a)  $n_0$  is an exterior node;
- (b)  $n_1, n_2, \dots, n_{k-1}$  are interior nodes;
- (c) there is a sequence  $G_0, G_1, \dots, G_k$  of weighted graphs  $G_i = (N, E, w_i)$  which can be constructed as follows:

- (c1)  $G_0 = G$ ;
- (c2) for  $i = 0, 1, \dots, k-2$  the graph  $G_{i+1} = (N, E, w_{i+1})$  is defined if and only if  $G_i$  is defined and  $|w_i(n_i, n_{i+1}) - w_i(n_{i+1}, n_{i+2})| = 1$ . In this case,

$$w_{i+1}(n, n') = \begin{cases} w_i(n, n'), & \text{if } (n, n') \neq (n_i, n_{i+1}) \\ 3 - w_i(n_i, n_{i+1}), & \text{if } (n, n') = (n_i, n_{i+1}) \end{cases}$$

for all  $n, n' \in N$ .

- (c3)  $G_k$  is defined if and only if  $G_{k-1}$  is defined. In this case,

$$w_k(n, n') = \begin{cases} w_{k-1}(n, n'), & \text{if } (n, n') \neq (n_{k-1}, n_k) \\ 3 - w_{k-1}(n_{k-1}, n_k), & \text{if } (n, n') = (n_{k-1}, n_k) \end{cases}$$

for all  $n, n' \in N$ .

Such a partial soliton path is called a (*total*) *soliton path* if  $n_k$  is an exterior node.

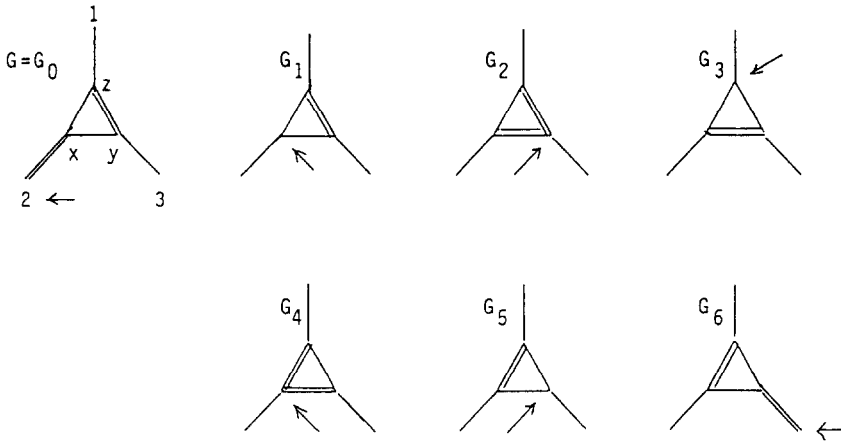


FIG. 4. Example of a soliton path and the corresponding sequence of graphs.

The example in Fig. 4 illustrates the definition of a soliton path.  $G_0$  is the initial graph. We then consider the path  $2xyzxy3$  resulting in the sequence  $G_1, \dots, G_6$  of graphs. In each of them the "position of the soliton" is indicated by an arrow. Note that the intermediate graphs  $G_1, \dots, G_5$  are not necessarily soliton graphs. For the interpretation again one has to keep in mind that single edges in the graph may well represent more complex structures—like long chains, for instance; this would have an effect on the timing of such a system.

Given a soliton graph  $G = (N, E, w)$  and a pair of exterior nodes  $n, n' \in N$ , let  $S(G, n, n')$  be the set of weighted graphs  $G'$  which can be obtained as  $G' = G_k$  according to the construction given in Definition 3.2 for some soliton path  $n = n_0, \dots, n_k = n'$ . We say that  $G'$  is generated by a transition from  $G$  if  $G' \in S(G, n, n')$  for some exterior nodes  $n, n' \in N$ .

The following lemma states that our definitions so far make sense.

**LEMMA 3.3.** *Let  $G$  be a soliton graph, and let  $G' \in S(G, n, n')$  for some exterior nodes of  $G$ . Then also  $G'$  is a soliton graph.*

*Proof.* Let  $n_0 = n, n_1, \dots, n_k = n'$  be a soliton path such that  $G' = G_k$  with  $G_0, G_1, \dots, G_k$  as in Definition 3.2. As only the weight function is affected by the transition from  $G_0$  to  $G_k$ , conditions (a–c) of Definition 3.1 hold true trivially for  $G_k$ . To prove (d) and (e) observe that

$$w_i(n_i, n_{i+1}) + w_i(n_{i+1}, n_{i+2}) = w_{i+2}(n_i, n_{i+1}) + w_{i+2}(n_{i+1}, n_{i+2})$$

for  $i = 0, \dots, k-2$ , and thus

$$w_i(n_{i+1}) = w_{i+2}(n_{i+1}).$$

By (a),  $n_i \neq n_{i+2}$ . Together this implies (d) and (e) for  $k > 1$ ; the case of  $k \leq 1$  is obvious. ■

As an immediate consequence of the definitions one obtains the statement:

**LEMMA 3.4.** *Let  $G$  be a soliton graph, and let  $n_0, n_1, \dots, n_k$  be a soliton path of  $G$ . Then also  $n_k, n_{k-1}, \dots, n_0$  is a soliton path of  $G$ . Thus, if  $G'$  is obtained from  $G$  by a transition, then also  $G$  is obtained from  $G'$  by a transition.*

For a set of soliton graphs  $\mathcal{G}$  consider the sequence  $\mathcal{G}_0 = \mathcal{G}, \mathcal{G}_1, \mathcal{G}_2, \dots$ , where for  $i = 0, 1, 2, \dots$ , the set  $\mathcal{G}_{i+1}$  is the union of  $\mathcal{G}_i$  with the set of those soliton graphs which can be obtained by a transition from a graph in  $\mathcal{G}_i$ . The particular case of interest in this paper is that of  $\mathcal{G} = \{G\}$ . In this case let

$$S(G) = \bigcup_{i=0}^{\infty} \mathcal{G}_i.$$

Obviously, as  $G$  is finite, also  $S(G)$  is finite and, in fact, can be obtained in finitely many computational steps.

**LEMMA 3.5.** *Let  $G$  be a soliton graph, and let  $G' \in S(G)$ . Then  $S(G') = S(G)$ .*

*Proof.* By the definition of  $S(G)$  one has  $S(G') \subseteq S(G)$ . The converse follows from Lemma 3.4. ■

We are now ready for the central definition of this paper:

**DEFINITION 3.6.** Let  $G$  be a soliton graph with  $X$  its set of exterior nodes. The *soliton automaton* based on  $G$  is defined as the non-deterministic automaton

$$\mathcal{A}(G) = (S(G), X \times X, \delta)$$

subject to the conditions:

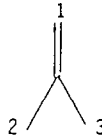
- (a)  $S(G)$  is the set of states;
- (b)  $X \times X$  is the input alphabet;
- (c)  $\delta: S(G) \times X \times X \rightarrow 2^{S(G)}$  is the transition function with

$$\delta(G', n, n') = \begin{cases} S(G', n, n'), & \text{if } S(G', n, n') \neq \emptyset \\ \{G'\}, & \text{otherwise} \end{cases}$$

for  $G' \in S(G)$  and  $n, n' \in X$ .

Usually, a soliton automaton will have several equivalent input symbols, that is, input symbols which cause exactly the same state transitions. For instance, the symbols  $(n, n')$  and  $(n', n)$  for  $n, n' \in X$  are always equivalent. In the sequel, such equivalent inputs will not be mentioned explicitly.



FIG. 5. Graph  $G$  of Example 3.7.

Note that the empty path is never considered a soliton path. Hence, if  $n$  is an exterior node the set  $S(G, n, n)$  resulting from soliton paths starting and ending at  $n$  will be non-empty only if there are non-empty cyclic soliton paths from  $n$  to itself. Otherwise, the transition caused by  $(n, n)$  is defined as the identity transition. Let us study some examples.

EXAMPLE 3.7. Consider the graph  $G$  shown in Fig. 5. One obtains the transitions as shown in Fig. 6. The resulting automaton  $\mathcal{A}_1$  has the transition function:

	$a$	$b$	$c$
$(1, 2)$	$b$	$a$	$c$
$(1, 3)$	$c$	$b$	$a$
$(2, 3)$	$a$	$c$	$b$

EXAMPLE 3.8. Consider the graph  $G$  of Fig. 7; one obtains the transitions as shown in Fig. 8. Note the following fact: The transition in the left column uses the path  $1zy3$  from 1 to 3, whereas in the right column the path used is  $1zxy3$ . The paths on the diagonal are  $2xzy3$  and  $2xyzxy3$ . The resulting automaton  $\mathcal{A}_2$  has the transition function:

	$a$	$b$	$c$	$d$
$(1, 2)$	$b$	$a$	$d$	$c$
$(1, 3)$	$d$	$c$	$b$	$a$
$(2, 3)$	$c$	$d$	$a$	$b$

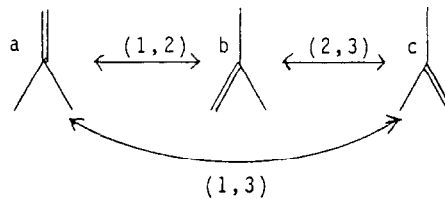


FIG. 6. Transitions for Example 3.7.

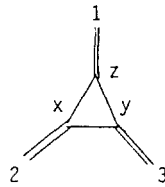


FIG. 7. Graph  $G$  of Example 3.8.

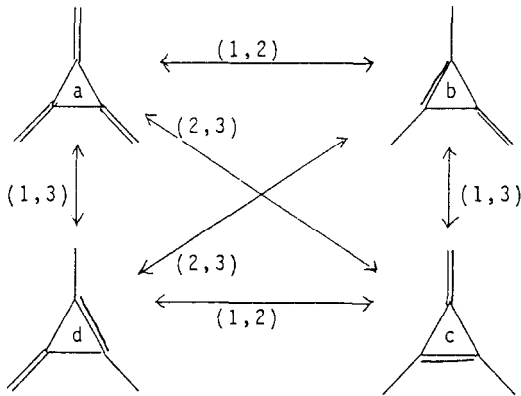


FIG. 8. Transitions for Example 3.8.

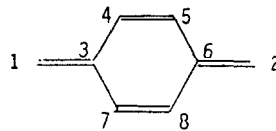


FIG. 9. Graph  $G$  of Example 3.9.

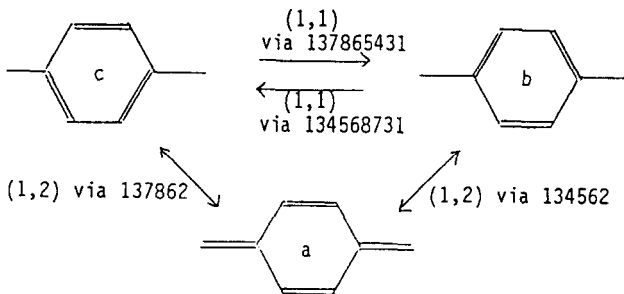


FIG. 10. Transitions for Example 3.9.

EXAMPLE 3.9. Consider the graph  $G$  of Fig. 9. One obtains the transitions as shown in Fig. 10. The resulting automaton  $\mathcal{A}_3$  has the transition function:

	$a$	$b$	$c$
$(1, 1)$	$a$	$c$	$b$
$(1, 2)$	$b, c$	$a$	$a$

The automaton  $\mathcal{A}_3$  is non-deterministic in the usual sense of the term. However, it also exhibits a slightly different kind of non-determinism—as does  $\mathcal{A}_2$ : For the same input symbol different paths can be used which, nevertheless, result in the same state transition. This distinction is made precise in the following definition:

DEFINITION 3.10. Let  $G$  be a soliton graph.  $G$  is called *deterministic* if  $|S(G', n, n')| \leq 1$  for all  $G' \in S(G)$  and all exterior nodes  $n, n' \in N$ . It is called *strongly deterministic* if for every  $G' \in S(G)$  and for every pair of exterior nodes  $n, n' \in N$  there is at most one soliton path from  $n$  to  $n'$  in  $G'$ .

It is obvious that determinism and strong determinism are decidable properties of soliton graphs. More detailed statements are proved in the sequel.

From a physico-chemical point of view, the notion of deterministic soliton graphs seems to be more natural than its restriction to strong determinism. However, for mathematical reasons we focus on strongly deterministic soliton graphs in most of this paper.

Observe that the soliton automaton  $\mathcal{A}(G)$  based on a soliton graph  $G$  is deterministic in the usual automaton theoretic sense if and only if  $G$  is deterministic. By slight abuse of definitions, the soliton automaton  $\mathcal{A}(G)$  is called *strongly deterministic* if  $G$  is strongly deterministic.

#### 4. DECOMPOSITION OF SOLITON GRAPHS

Obviously the connected components of a soliton graph act as “independent units” in the corresponding soliton automaton. To be more precise, we state the following simple fact:

FACT 4.1. Let  $G$  be a soliton graph, and let  $G_1, \dots, G_r$  be its connected components. Then  $\mathcal{A}(G)$  and  $\prod_{i=1}^r \mathcal{A}(G_i)$  are isomorphic automata, and consequently,  $T(\mathcal{A}(G)) \simeq \prod_{i=1}^r T(\mathcal{A}(G_i))$ .

However, connectedness is insufficient as a property to guarantee that the resulting automaton be without such “independent subunits.” Indeed, such independent subunits exist whenever a connected soliton graph  $G$  contains subgraphs  $G_1$  and  $G_2$

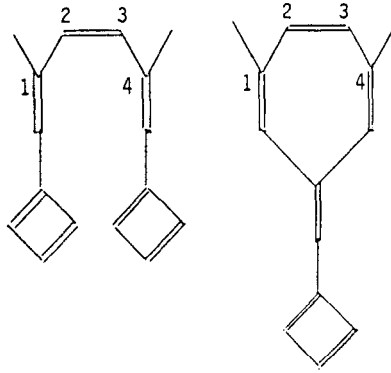


FIG. 11. Soliton graphs with impervious paths.

which are not joined by any soliton path. The notion of connectedness corresponding to this type of situation is studied in the present section.

**DEFINITION 4.2.** Let  $G = (N, E, w)$  be a soliton graph. An edge  $(n, n') \in E$  is said to be *impervious* if it is not contained in any partial soliton path of  $G$ . A path of  $G$  is called *impervious* if each of its edges is.

In Fig. 11 we show two examples of soliton graphs; in each the path 1234 is impervious.

**LEMMA 4.3.** Let  $G = (N, E, w)$  be a connected soliton graph, and let  $n_0, n_1, \dots, n_k$  with  $k > 0$  be an impervious path of  $G$ . Then also the path  $n_k, \dots, n_1, n_0$  is impervious. Furthermore, there are  $s, t \in \mathbb{N}_0$  and nodes  $m_0, \dots, m_s, p_0, \dots, p_t \in N$  which satisfy the conditions:

- (a)  $m_s = n_0$  and  $n_k = p_0$ ;
- (b) the path

$$m_0, \dots, m_s = n_0, \dots, n_k = p_0, \dots, p_t$$

is also impervious and has  $d(m_0) = d(p_t) = 3$ .

*Proof.* The first assertion is obvious. For the second statement, observe that neither  $n_0$  nor  $n_k$  can be exterior nodes. Therefore,  $d(n_0) \geq 2$  and  $d(n_k) \geq 2$ . Assume now that  $d(n_0) = 2$ . Then there exists a unique edge  $(m, n_0) \in E$  into  $n_0$  with  $m \neq n_1$ . This implies

$$|w(m, n_0) - w(n_0, n_1)| = 1.$$

If  $(m, n_0)$  were not impervious then it would form part of a partial soliton path,

$$u_0, u_1, \dots, u_r, m, n_0,$$

say, and thus also  $(n_0, n_1)$  would not be impervious—a contradiction! In this way we have shown that the path may be extended by the impervious edge  $(m, n_0)$  if  $d(n_0)=2$ . Applying this argument to  $n_0$  and to  $n_k$  inductively proves the statement. ■

By Lemma 4.3 an impervious path can always be extended—if necessary—to end and begin with nodes of degree three. A path  $n_0, n_1, \dots, n_k$  is a *basic impervious path* if  $d(n_0)=d(n_k)=3$  and  $d(n_1)=\dots=d(n_{k-1})=2$ . The next lemma shows that basic impervious paths can be omitted from a soliton graph without affecting its behaviour as an automaton.

**LEMMA 4.4.** *Let  $G=(N, E, w)$  be a deterministic soliton graph containing a basic impervious path  $n_0, \dots, n_k$ . Let*

$$\begin{aligned} N' &= N \setminus \{n_1, \dots, n_{k-1}\}, \\ E' &= E \setminus \{(n_0, n_1), (n_1, n_2), \dots, (n_{k-1}, n_k)\}, \end{aligned}$$

*and let  $w'$  be the restriction of  $w$  to  $E'$ . Then  $G'=(N', E', w')$  is a soliton graph satisfying  $T(\mathcal{A}(G)) \simeq T(\mathcal{A}(G'))$ .*

*Proof.* It is obvious that  $G'$  is a soliton graph. If  $H \in S(G)$  then the path  $n_0, \dots, n_k$  is impervious in  $H$  as well. Let  $H'$  be the graph obtained from  $H$  using the construction of the Lemma. Clearly,

$$S(G') = \{H' \mid H \in S(G)\},$$

and  $G$  and  $G'$  have the same set  $X$  of exterior nodes and the same soliton paths. Let  $\mathcal{A}=(S(G), X \times X, \delta)$  and  $\mathcal{A}'=(S(G'), X \times X, \delta')$  be the soliton automata based on  $G$  and  $G'$ , respectively. Then the mapping

$$\delta_{(n, m)} \mapsto \delta'_{(n, m)}$$

induces an isomorphism of  $T(\mathcal{A})$  onto  $T(\mathcal{A}')$ . ■

Let  $G$  be a soliton graph. Using the construction of the lemma on its connected components iteratively, one obtains a *reduced soliton graph*  $H$  with the same set  $X$  of exterior nodes such that the connected components  $H_1, \dots, H_r$  of  $H$  themselves contain no basic impervious paths. Indeed,  $H$  is uniquely determined by  $G$ . The decomposition  $H_1, \dots, H_r$  of  $H$  is called the *soliton decomposition* of  $G$ . By induction one obtains the following result from Lemma 4.4.

**PROPOSITION 4.5.** *Let  $G$  be a soliton graph with soliton decomposition  $G_1, \dots, G_r$  and with set  $X$  of exterior nodes.*

(a) *The mapping*

$$S(G) \rightarrow S(G_1) \times \dots \times S(G_r): H \mapsto (H_1, \dots, H_r)$$

with a suitably fixed ordering of the components induces an automaton isomorphism of  $\mathcal{A}(G)$  onto  $\prod_{i=1}^r G_i$ .

(b) The identity mapping on  $X \times X$  induces an isomorphism of  $T(\mathcal{A}(G))$  onto  $\prod_{i=0}^r T(\mathcal{A}(G_i))$ .

A soliton graph is called *indecomposable* if it is connected and contains no imperious edges. By Proposition 4.5 every soliton automaton is isomorphic with a product of soliton automata based on indecomposable soliton graphs; furthermore, the transition monoid of a soliton automaton is isomorphic with a direct product of transition monoids of soliton automata based on indecomposable soliton graphs.

## 5. STRONGLY DETERMINISTIC SOLITON GRAPHS

In this section we give a partial characterization of the transition semigroups of soliton automata based on strongly deterministic soliton graphs. From these results it follows, in particular, that not every finite automaton can be simulated by a soliton automaton.

Our first result states that the presence of a cycle of odd length implies that  $G$  is not strongly deterministic.

**PROPOSITION 5.1.** *Let  $G = (N, E, w)$  be a soliton graph and let  $n_0, \dots, n_i, \dots, n_k$  be a partial soliton path of  $G$  with the properties:*

- (1)  $k - i$  is odd;
- (2)  $n_i = n_k$ ;
- (3)  $n_j \neq n_l$  for  $i \leq j < l < k$ .

*Then  $G$  is not strongly deterministic and  $G \in S(G, n_0, n_0)$ .*

*Proof.* From the definition of soliton graphs it follows that  $k - i > 1$  and therefore  $d(n_i) \geq 2$ . Thus,  $n_i$  is interior, hence  $i > 0$  from the definition of partial soliton paths. Under these conditions the only way to assign weights to the edges around  $n_i$  is as follows:

$$\begin{aligned} w(n_{i-1}, n_i) &= 2, \\ w(n_i, n_{i+1}) &= 1, \\ w(n_j, n_{j+1}) + w(n_{j+1}, n_{j+2}) &= 3 \end{aligned}$$

for  $j = i, \dots, k - 2$ , and

$$w(n_{k-1}, n_k) = 1.$$

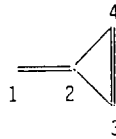


FIG. 12. Soliton graph with a cycle of odd length.

To prove the statement we merely observe that this situation allows for two different soliton paths:

$$n_0, \dots, n_i, n_{i+1}, \dots, n_{k-1}, n_k = n_i, n_{i+1}, \dots, n_{k-1}, n_k = n_i, n_{i-1}, \dots, n_0$$

and

$$n_0, \dots, n_i = n_k, n_{k-1}, \dots, n_{i+1}, n_i = n_k, n_{k-1}, \dots, n_{i+1}, n_i, n_{i-1}, \dots, n_0.$$

This also shows that  $G \in S(G, n_0, n_0)$ . ■

In Fig. 12 we display a typical example of a soliton graph with a cycle of odd length.

Arguments similar to those in the above proof are insufficient, however, to show also that the presence of cycles of even length is impossible for strongly deterministic soliton graphs. Indeed, it turns out that strongly deterministic indecomposable soliton automata with cycles of even lengths exist. However, they are of a quite restricted kind. As a typical example consider the graph shown in Fig. 13 which has a cycle of length 4. This graph is strongly deterministic, its soliton automaton has two states, and the transition monoid is the symmetric group  $\mathcal{S}_2$  on this state set.

**PROPOSITION 5.2.** *Let  $G$  be a deterministic indecomposable soliton graph containing a path  $n_0, n_1, \dots, n_k$  satisfying the following conditions:*

- (1)  $k$  is even and  $k > 0$ ;
- (2)  $n_0 = n_k$ ;
- (3)  $n_j \neq n_l$  for  $0 \leq j < l < k$ ;
- (4)  $w(n_j, n_{j+1}) + w(n_{j+1}, n_{j+2}) = 3$  for  $j = 0, \dots, k-2$ .

*Then  $T(\mathcal{A}(G))$  is  $\mathcal{S}_2$ , the symmetric group on 2 elements.*

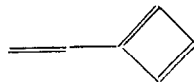
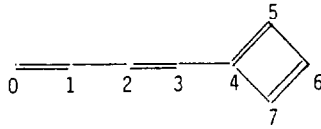


FIG. 13. Strongly deterministic soliton graph with a cycle of even length.


 FIG. 14. Graph  $G_1$  in the proof of Proposition 5.2.

*Proof.* Let  $X$  be the set of exterior nodes of  $G$ , and let  $v = |X|$ . We use induction on  $v$ .

*Case  $v = 1$ .* Let  $v = 1$ . As  $G$  is indecomposable there is a partial soliton path containing at least one of the edges  $(n_i, n_{i+1})$  with  $0 \leq i < k$ . Therefore, up to length of the cycle and the length of the partial soliton path leading into the cycle we may assume—without loss in generality—that  $G$  has a subgraph  $G_1$  of the whose shape is shown in Fig. 14. There is a soliton path 0123456743210 which results in a transition to the subgraph  $G_2$  as shown in Fig. 15 with the rest of  $G$  unaffected: Let  $G'$  be the graph obtained from  $G$  in this manner. Clearly,  $G' \in S(G, 0, 0)$  and  $G \in S(G', 0, 0)$ .

If  $G = G_1$  then  $G$  is strongly deterministic with  $S(G) = \{G, G'\}$  and with  $(0, 0)$  acting as the non-trivial permutation of  $S(G)$ .

We now show that as a deterministic soliton graph  $G$  cannot have any further edges except of a very special kind; and in that case  $T(\mathcal{A}(G)) \simeq \mathcal{S}_2$ .

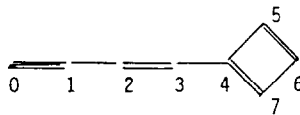
Suppose,  $(x, y)$  is an edge of  $G$  not contained in  $G_1$ . As  $v = 1$ , any partial soliton path containing  $(x, y)$  will have an initial segment  $x_1, x_2, \dots, x_n$  which satisfies one of the following conditions:

- (1) for some  $i \in \{1, 2\}$  and some  $j$  the path  $x_1, x_2, \dots, x_j$  is in  $G_i$ ; the nodes  $x_j, \dots, x_{n-1}$  are distinct; the nodes  $x_{j+1}, \dots, x_{n-1}$  do not belong to  $G_i$ ; for some  $k$  with  $j+1 \leq k < n-1$  one has  $x_n = x_k$ ;
- (2) for some  $i \in \{1, 2\}$  and some  $j$  the path  $x_1, x_2, \dots, x_j$  is in  $G_i$ ; the nodes  $x_j, \dots, x_{n-1}$  are distinct; the nodes  $x_{j+1}, \dots, x_{n-1}$  are not in  $G_i$ ;  $x_n$  belongs to  $G_i$ .

In case (1) there is an additional cycle completely outside  $G_i$  as illustrated in Fig. 16. In case (2) again there is an additional cycle which, however, uses part of  $G_i$ . The twelve possible situations are shown in Fig. 17.

*Case (1).* If the additional cycle has odd length then, by the previous proposition, one has

$$\{G, G'\} \subseteq S(G, 0, 0) \quad \text{with} \quad G \neq G',$$


 FIG. 15. Graph  $G_2$  in the proof of Proposition 5.2.



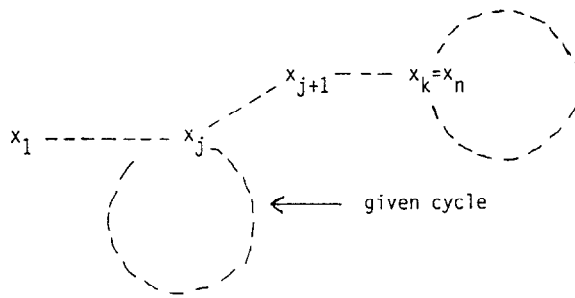


FIG. 16. Case (1) in the proof of Proposition 5.2.

and  $G$  is not deterministic. If it has even length, then, as has been shown before for the given cycle, there is a soliton path which changes all weights in that additional cycle and leaves the rest of  $G$  unchanged. The resulting soliton graph  $G''$  is different from  $G'$  and

$$\{G', G''\} \subseteq S(G, 0, 0),$$

again a contradiction.

*Case (2).* As the path  $x_j, \dots, x_n$  begins and ends with an edge of weight 1, its length has to be odd. In the situations (a-c) and (i-k) of Fig. 17 there is a soliton path satisfying the assumptions of the previous proposition. Therefore, in these situations one has

$$\{G, G'\} \subseteq S(G, 0, 0) \quad \text{with} \quad G \neq G',$$

contradicting determinism. In the situations (d), (f-h), and (l) there is a cycle of even length different from the given one and contained in a soliton path. As in case (1) the set  $S(G, 0, 0)$  contains at least two elements, again a contradiction! Finally in situation (e), there are two different paths for input  $(0, 0)$  which result in different transitions. Thus  $G$  is not deterministic.

This proves the statement for the case  $v = 1$ .

*Case  $v > 1$ .* Let  $v > 1$ . We assume that the statement holds true for all soliton graphs with fewer than  $v$  exterior nodes. Let  $G$  be a soliton graph satisfying the assumptions and having  $v$  exterior nodes.

As in the case of  $v = 1$  we may assume the existence of a soliton path using a subgraph  $G_1$  of the shape shown in Fig. 14. Using the same notation as above one finds that

$$G' \in S(G, 0, 0) \quad \text{and} \quad G \in S(G', 0, 0).$$

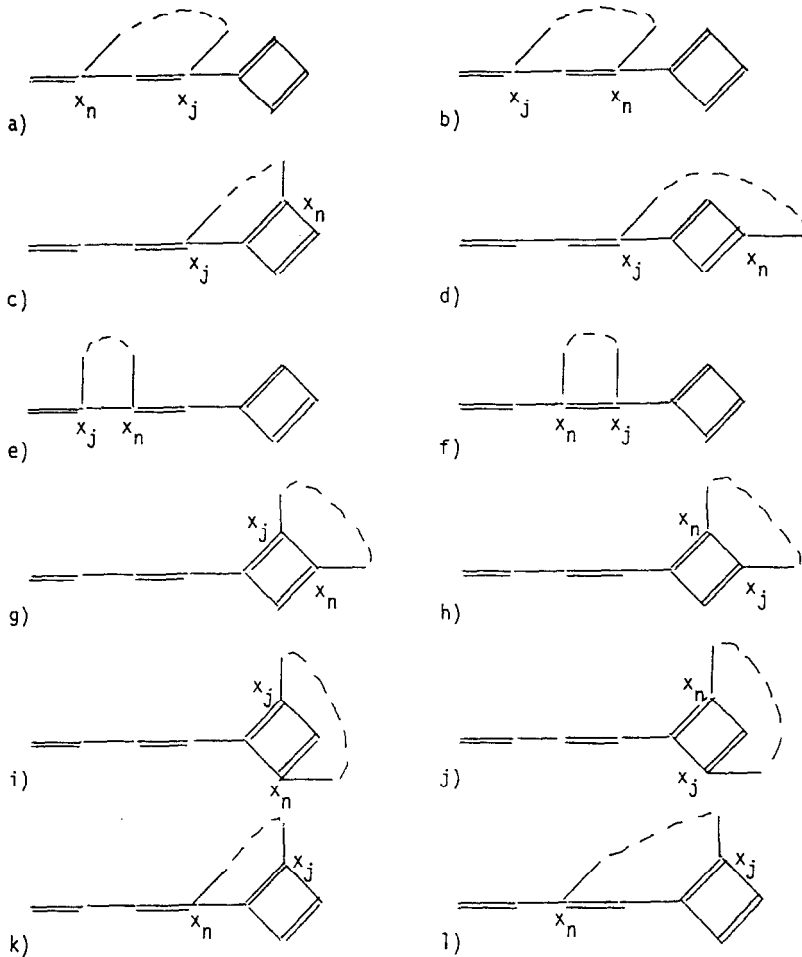


FIG. 17. Case (2) in the proof of Proposition 5.2.

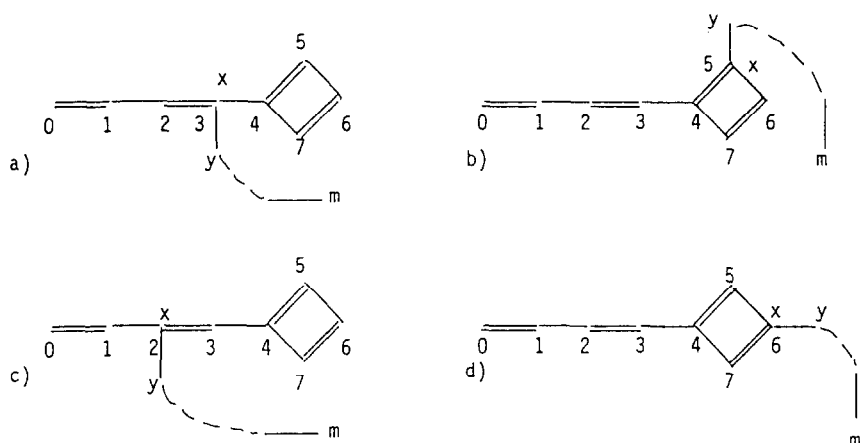
Indeed, by the previous case, these are the only possibilities. Now consider an additional edge  $(x, y)$  with  $x$  in  $G_1$  which is on a partial soliton path starting with some exterior node  $m$ ,  $m \neq 0$ . The existence of such an edge follows from the assumption of indecomposability.

There are four cases. The typical situations are illustrated in Figure 18.

*Case (a).* The input  $(0, m)$  allows for two different soliton paths

$$0, 1, 2, 3 = x, y, \dots, m \quad \text{and} \quad 0, 1, 2, 3, 4, 5, 6, 7, 4, 3 = x, y, \dots, m$$

leading to different soliton graphs, a contradiction!

FIG. 18. Case  $v > 1$  in the proof of Proposition 5.2.

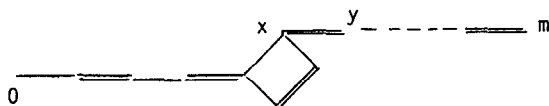
*Case (b).* Using input  $(0, m)$  once results in the soliton graph  $G''$  shown in Fig. 19. Now,  $G''$  contains two soliton paths for input  $(0, m)$  which again lead to different soliton graphs, a contradiction!

*Cases (c–d).* In these cases as far as the subgraph shown is concerned, each soliton path starting at 0 or at  $m$  returns to its origin. Furthermore, either will change  $G$  into  $G'$  and vice versa. By cases (a–b) this obtains for all exterior nodes  $m$  of  $G$  with which 0 is connected at all. Now, we eliminate the node 0 and further nodes  $x_1, \dots, x_{r-1}$  forming a path

$$0, x_1, \dots, x_r \quad \text{with} \quad d(x_1) = \dots = d(x_{r-1}) = 2.$$

Let  $H$  be the resulting soliton graph. Then  $H$  contains the given cycle, has fewer than  $v$  exterior nodes, and has  $T(\mathcal{A}(H)) \simeq T(\mathcal{A}(G))$ . This proves  $T(\mathcal{A}(G)) \simeq \mathcal{L}_2$ . ■

An indecomposable soliton graph which consists of a single cycle of even length and some paths leading into it—as shown in Fig. 20—is called a *chestnut* in the sequel. The only condition on the way in which the paths enter the cycle is: Entry points of different paths entering the cycle haven even distance; paths leading to the cycle may meet only at even distances from entry into the cycle.

FIG. 19. Graph  $G''$  in the proof of Proposition 5.2.

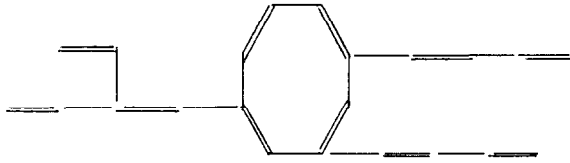


FIG. 20. Chestnut.

From the proof of Proposition 5.2 one derives the following statement.

**COROLLARY 5.3.** *Let  $G$  be a strongly deterministic indecomposable soliton graph containing a path  $n_0, n_0, \dots, n_k$  satisfying the conditions:*

- (1)  $k$  is even and  $k > 0$ ;
- (2)  $n_0 = n_k$ ;
- (3)  $n_j \neq n_l$  for  $0 \leq j < l < k$ ;
- (4)  $w(n_j, n_{j+1}) + w(n_{j+1}, n_{j+2}) = 3$  for  $j = 0, \dots, k-2$ .

*Then  $G$  is a chestnut.*

*Proof.* In the previous proof the soliton graphs which are different from chestnuts are shown to be non-deterministic or turn out to be not strongly deterministic. ■

We combine these results to obtain the following characterization of strongly deterministic indecomposable soliton graphs.

**PROPOSITION 5.4.** *Let  $G = (N, E, w)$  be an indecomposable soliton graph. Then  $G$  is strongly deterministic if and only if  $G$  is a chestnut or  $(N, E)$  is a tree.*

*Proof.* If  $G$  is an indecomposable soliton graph with  $G$  a chestnut or  $(N, E)$  a tree then  $G$  is strongly deterministic. To prove the converse, assume that  $G$  is a strongly deterministic indecomposable soliton graph with  $(N, E)$  not a tree. Then there is a cycle  $n_0, \dots, n_k$  of length  $k > 2$  in  $(N, E)$  with  $n_0 = n_k$  and  $n_j \neq n_l$  for  $0 \leq j < l < k$ . To complete the proof we have to show that this implies that for some  $G' \in S(G)$  there is a cycle (possibly a different one) which forms the tail end of a partial soliton path in  $G'$ . In this case, if that cycle has odd length, the graph is not strongly deterministic, and if it has even length then  $G$  is a chestnut. The difficulty lies in the fact that we cannot assume that the cycle  $n_0, \dots, n_k$  has edges with alternating weights. However, as  $G$  is indecomposable we know that there is a partial soliton path containing an edge of this cycle; with loss in generality, let

$$m_0, \dots, m_r = n_0, n_1$$

be such a path. Now extend this partial soliton path as far as possible along the cycle, that is, as far as it still is a partial soliton path yielding

$$m_0, \dots, m_r = n_0, n_1, \dots, n_s.$$

If  $s = k$  we have a soliton path from  $m_0$  to  $m_0$  containing a cycle of length  $k$ . If  $k$  is odd then  $G$  is not strongly deterministic, a contradiction! If  $k$  is even then  $G$  is a chestnut.

Assume now that  $s < k$ , that is,  $w(n_{s-1}, n_s) = w(n_s, n_{s+1}) = 1$ . As  $G$  is a soliton graph there is a node  $p_1$  and an edge  $(n_s, p_1)$  with weight 2. Therefore, also

$$m_0, \dots, m_r = n_0, n_1, \dots, n_s = p_0, p_1$$

is a partial soliton path. Extend this path until one of the following conditions is satisfied:

- (1) a node already on the path is reached again;
- (2) an exterior node is reached;
- (3) a node on the cycle  $n_0, \dots, n_k$  is reached.

Let

$$m_0, \dots, m_r = n_0, n_1, \dots, n_s = p_0, p_1, \dots, p_t$$

be the resulting partial soliton path.

In case (1), this path contains a cycle, and the above argument applies again.

In case (2), using this path with input  $(m_0, p_t)$  results in a soliton graph  $G'$  with weight function  $w'$  such that

$$m_0, \dots, m_r = n_0, n_1, \dots, n_s$$

is a partial soliton path of  $G'$ ,

$$w'(n_{s-1}, n_s) = 2$$

and

$$w'(n_s, n_{s+1}) = 1.$$

Therefore, also

$$m_0, \dots, m_r = n_0, n_1, \dots, n_s, n_{s+1}$$

is a partial soliton path of  $G'$  containing one more edge of the original cycle.

In case (3), letting  $p_t = n_j$ , one extends the path by one of the edges  $(n_j, n_{j-1})$  or  $(n_j, n_{j+1})$  of the cycle.

Iterating this construction at most  $k$  times will result in a soliton path containing a cycle. This was to be proved. ■

## 6. STRONGLY DETERMINISTIC SOLITON AUTOMATA AND THEIR TRANSITION MONOIDS

From the fact that every soliton transition induces an involutorial mapping it is obvious that only groups are possible as transition monoids of soliton automata.

We now give a more detailed description of the corresponding class of groups. In particular, we prove that it is rich enough so that every automaton whose transition monoid is a group can be simulated by a soliton automaton.

In the previous section we showed that every strongly deterministic soliton automaton is the sum of a family of strongly deterministic automata which are based on indecomposable strongly deterministic soliton graphs. Thus their transition monoids are direct products of the transition monoids of such components. As components only chestnuts or trees are possible. The soliton automata of chestnuts are 2-state automata with a single input symbol whose transition monoid always is the symmetric group  $\mathcal{S}_2$  on two elements. It remains to study the transition monoids of soliton automata based on trees.

Let  $(N, E)$  be a graph. Any soliton graph  $(N, E, w)$  is called a *soliton graph interpretation* of  $(N, E)$ . Let  $\Sigma(N, E)$  denote the set of all soliton graph interpretations of  $(N, E)$ . A soliton graph  $G = (N, E, w)$  is said to be a *soliton tree* if  $(N, E)$  is a tree. First we show that a tree always has a unique soliton automaton associated with it.

**PROPOSITION 6.1.** *Let  $(N, E)$  be a binary tree and let  $G$  be any soliton graph interpretation of  $(N, E)$ . Then  $S(G) = \Sigma(N, E)$ .*

*Proof.* We use induction on the number  $v$  of exterior nodes (leaves) of the tree. Inspection of all cases shows that the statement is true for  $v = 2$  and  $v = 3$ . Now, assume that  $v > 3$  and that the assertion holds for all trees with fewer than  $v$  exterior nodes. Let  $G = (N, E, w)$  be a soliton tree with  $v$  exterior nodes. Consider an exterior node  $n_0 \in N$  such that there is a path in  $(N, E)$  which originates at  $n_0$  and contains exactly one node of degree 3. This path need not be a soliton path! Obviously, such a path exists. Without loss in generality we can assume that it is of the form:

$$n_0, n_1, n_2.$$

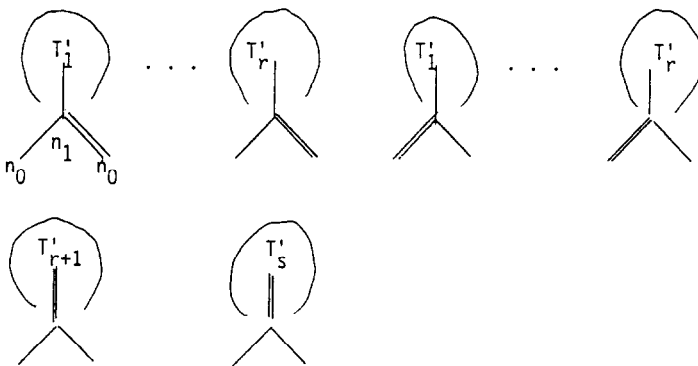


FIG. 21. Soliton tree expansions of  $T'$  in Proposition 6.1.



FIG. 22. Soliton trees used in the proof of Proposition 6.2.

Our next result describes the transition monoids of soliton trees. For this we review a few group theoretic terms.

Let  $\mathcal{G}$  be a permutation group on a set  $\Omega$ . A subset  $\Psi$  of  $\Omega$  is called a *block* if for each  $g \in \mathcal{G}$  the image  $\Psi^g$  either coincides with  $\Psi$  or is disjoint from  $\Psi$ . The sets  $\emptyset$ ,  $\{\omega\}$  for  $\omega \in \Omega$ , and  $\Omega$  are the *trivial blocks*. The group  $\mathcal{G}$  is called *primitive* if it is transitive and has only trivial blocks.

**PROPOSITION 6.2.** *Let  $G$  be a soliton tree. Then  $T(\mathcal{A}(G))$  is a primitive permutation group.*

*Proof.* The proof uses induction on the number  $v$  of exterior nodes (leaves) of the tree. Obviously, for  $v=2$  there is a single soliton automaton only, and its transition monoid is the symmetric group  $\mathcal{S}_2$ . The symmetric groups are known to be primitive.

Now let  $G = (N, E, w)$  be a soliton tree with  $v$  exterior nodes,  $v > 2$ , and assume that the assertion is true for all soliton trees with fewer than  $v$  exterior trees. Fix some arbitrary numbering of the exterior nodes of  $G$  from 1 to  $v$  subject to the condition that there is a path (not necessarily soliton) from  $v-1$  to  $v$  which contains exactly one node of degree 3. Without loss in generality we can assume that this path is of length 2 and has one of the three forms shown in Fig. 22. Let  $H$  be the soliton graph obtained from  $G$  by omitting the nodes  $v-1$  and  $v$ . The “new” exterior node in  $H$  gets the number  $v-1$ .

As in the previous proof consider the soliton trees generated starting from  $H$ . Number them in such a way that

$$H_1, H_2, \dots, H_k$$

are those with a weight of 1 for the edge leading to node  $v-1$  and that

$$H_{k+1}, \dots, H_s$$

are those in which that edge has a weight of 2. Based on this enumeration one gets three classes of soliton trees with  $v$  exterior nodes:

$$\Omega_1 = \{G_1, \dots, G_k\}$$

are the soliton trees obtained from  $H_1, \dots, H_k$  by re-inserting two exterior nodes

with numbers  $v-1$  and  $v$  instead of  $v-1$  in such a way that the edges leading to  $v-1$  and  $v$  have the weights 2 and 1, respectively;

$$\Omega_2 = \{G'_1, \dots, G'_k\}$$

are obtained analogously with the weights switched. Finally,

$$\Omega_3 = \{G_{k+1}, \dots, G_s\}$$

are the trees obtained from  $H_{k+1}, \dots, H_s$  in this fashion with both weights equal to 1. By construction,

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 = \Sigma(N, E) = S(G).$$

We have to prove that  $T(\mathcal{A}(G))$  is a primitive group of permutations of  $\Omega$ .

Transitivity is obvious. Now let  $\Delta \subseteq \Omega$  with  $1 < |\Delta| < |\Omega|$ , and let

$$\Delta' = \Delta \cap (\Omega_1 \cup \Omega_3).$$

First assume that  $2 < |\Delta'|$  and  $\Delta' \neq \Omega_1 \cup \Omega_3$ . Let  $\Delta''$  be the set of soliton trees in  $S(H)$  from which the soliton trees in  $\Delta'$  have been constructed. By the assumptions one has  $2 < |\Delta''|$  and  $\Delta'' \neq S(H)$ . Using the induction hypothesis one concludes that there is a permutation  $g \in T(\mathcal{A}(H))$  with  $T_1^g \in \Delta''$  and  $T_2^g \notin \Delta''$  for some  $T_1', T_2' \in \Delta''$ . Note that the transitions of  $\mathcal{A}(H)$  have uniquely determined extensions to  $\Omega_1 \cup \Omega_3$ . Thus to  $g$  there corresponds a unique element of  $T(\mathcal{A}(G))$  also denoted by  $g$  which is generated by the extended transitions. Let  $T_1, T_2 \in \Delta'$  be the soliton trees extending  $T_1'$  and  $T_2'$ . Observe that they are uniquely determined by  $T_1'$  and  $T_2'$ , too. Then  $T_1^g \in \Delta'$  and  $T_2^g \notin \Delta'$ , and  $T_2^g \in \Omega_1 \cup \Omega_3$  implies  $T_1^g \in \Delta$  and  $T_2^g \notin \Delta$ . In this case  $\Delta$  is not a block.

If, on the other hand,  $\Delta' = \Omega_1 \cup \Omega_3$  then  $|\Delta'| > \frac{1}{2} |\Omega|$ . Thus,  $|\Delta'|$  is not a divisor of  $|\Omega|$ . By [14, Proposition 6.3] this implies that  $\Delta$  is not a block.

Now, let  $|\Delta'| = 1$ . In this case we replace  $\Delta'$  by  $\Delta \cap (\Omega_2 \cup \Omega_3)$  in the above arguments.

This leaves us with the case:

$$|\Delta \cap (\Omega_1 \cup \Omega_3)| = |\Delta \cap (\Omega_2 \cup \Omega_3)| = 1.$$

If  $\Delta' \subseteq \Omega_3$  then  $\Delta = \Delta'$  and  $|\Delta| = 1$ , a contradiction! Therefore, let  $\Delta \cap (\Omega_1 \cup \Omega_3) = \{T_1\} \subseteq \Omega_1$  and  $\Delta \cap (\Omega_2 \cup \Omega_3) = \{T_2\} \subseteq \Omega_2$ ; that is,  $\Delta = \{T_1, T_2\}$ . Let  $g \in T(\mathcal{A}(G))$  correspond to a transition from  $T_1$  which has  $v$  as its target node. Then  $T_1^g \in \Omega_3$  whereas  $T_2^g = T_2$ . Thus  $T_1^g \notin \Delta$  and  $T_2^g \in \Delta$ . Also in this case,  $\Delta$  is not a block. ■

Combining these results with well-known automaton theoretic facts yields the following description of the computational power of soliton automata.

**PROPOSITION 6.3.** *If  $\mathcal{A}$  is a strongly deterministic soliton automaton then  $T(\mathcal{A})$*



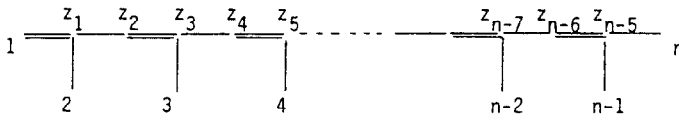


FIG. 23. Soliton tree  $G_n$  for Proposition 6.5.

is a direct product of primitive permutation groups which are generated by involutorial elements.

*Proof.*  $\mathcal{A}$  is the sum of its indecomposable components. For each of them the transition monoid is a primitive permutation group. Obviously, every input symbol induces a permutation of order 1 or 2. ■

**COROLLARY 6.4.** *Not every automaton can be simulated by a strongly deterministic soliton automaton.*

So far we have shown that the transition monoid of a strongly deterministic indecomposable soliton automaton is a primitive permutation group generated by involutorial elements. To give a more precise description of the class of groups involved remains an open problem. Our partial answer, which forms the subject of the rest of this section, states that this class contains the symmetric groups as well as some other groups.

**PROPOSITION 6.5.** *For every  $n \geq 2$  there is a soliton tree  $G_n$  such that  $T(\mathcal{A}(G_n)) = \mathcal{S}_n$ .*

*Proof.* Consider the soliton tree shown in Fig. 23. First we show that  $|\mathcal{S}(G_n)| = n$ . Let  $G \in \mathcal{S}(G_n)$ , and let  $k$  be an exterior node of  $G$  with  $w(k) = 2$ . Clearly, such  $G$  and  $k$  exist.

The typical shape of  $G$ —a consequence of the definition of soliton automata—is shown in Fig. 24. Thus, for each exterior node  $k$  the set  $\mathcal{S}(G_n)$  contains exactly one soliton tree with  $w(k) = 2$ .

Now observe that the input  $(1, n)$  induces a transposition on  $\mathcal{S}(G_n)$ . By [14, Theorem 13.3], the primitive group  $T(\mathcal{A}(G_n))$  is the symmetric group on  $\mathcal{S}(G_n)$ . ■

Obviously, the transition monoid of a soliton automaton is a group. The converse is an immediate consequence of Proposition 6.5.

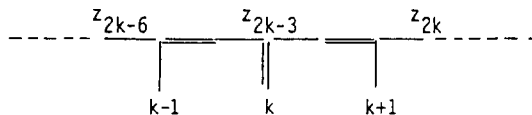
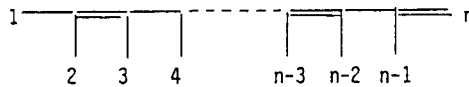


FIG. 24. Soliton tree  $G$  for Proposition 6.5.

FIG. 25. "Fibonacci tree"  $H_n$ .

COROLLARY 6.6. *An automaton can be simulated by a strongly deterministic soliton automaton if and only if its transition monoid is a group.*

Whereas the type of trees used in the proof of Proposition 6.5 requires  $\Omega(n)$  nodes to yield  $\mathcal{S}_n$  as the transition monoid, an infinite class of symmetric groups  $\mathcal{S}_n$  can be obtained with soliton trees having  $O(\log n)$  nodes only.

For  $n \geq 2$  consider the soliton tree  $H_n$  as shown in Fig. 25. One verifies that  $T(\mathcal{A}(H_n)) = \mathcal{S}_{F_n}$  where  $F_n$  is the  $n$ th Fibonacci number. It is well known that  $n = O(\log F_n)$ .

Our next example concerns a soliton tree  $G$  such that  $T(\mathcal{A}(G))$  is no symmetric group.  $G$  is shown in Fig. 26. By enumeration of all possibilities one finds that  $|\mathcal{S}(G)| = 12$  and that all permutations corresponding to soliton transitions are even. Therefore,  $T(\mathcal{A}(G))$  is a subgroup of the alternating group on 12 elements. Thus, considered as group of permutations, it is not symmetric. However, we could not rule out the possibility that  $T(\mathcal{A}(G))$  is isomorphic with a symmetric group. Extensive computation shows that it could only be isomorphic with  $\mathcal{S}_{10}$  or  $\mathcal{S}_{11}$  if this was the case at all. The order of  $T(\mathcal{A}(G))$  is known to exceed  $9!$ .

On the other hand, the alternating group  $\mathcal{A}_5$  of order 60 is a primitive permutation group generated by involutorial elements which is not the transition monoid of a strongly deterministic soliton automaton. As  $\mathcal{A}_5$  is not a direct product, any strongly deterministic soliton graph  $G$  with  $T(\mathcal{A}(G)) \simeq \mathcal{A}_5$  can be assumed to be a soliton tree. If the soliton tree is as in Fig. 11 or 12 then  $T(\mathcal{A}(G))$  is a symmetric group. Otherwise,  $G$  has to contain a subtree as shown in Fig. 13. But then the order of  $T(\mathcal{A}(G))$  is no less than that of the transition monoid belonging to the tree of Fig. 13, that is, no less than  $9!$ , and thus too large for  $\mathcal{A}_5$ .

In order to evaluate the statement of Corollary 6.6 one has to observe that the simulation of an automaton with a group as its transition monoid by a soliton automaton may be very costly, indeed. However, one should also note that the extent to which this problem is serious will also depend on the notion of simulation.

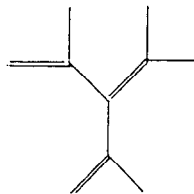


FIG. 26. Soliton tree.

First, the simulation is achieved via the embedding into a symmetric group at the cost of possibly "exploding" the number of states. However, one should keep in mind the above example showing that the "size" of a soliton tree for  $n$  states can be kept at  $O(\log n)$ .

Second, but no less important, the simulation requires an input encoding. That is, if  $X$  is the input alphabet of the automaton  $\mathcal{A}$  to be simulated and if  $Y$  is the set of exterior nodes of the soliton graph  $G$  simulating  $\mathcal{A}$  then in order to achieve corresponding transitions a morphism of  $X^*$  into  $(Y \times Y)^*$  is required as an input encoding. By arguments similar to those in [1] one shows that, asymptotically, the maximum length of input words over  $Y \times Y$  needed to generate all elements of  $\mathcal{S}_n$  has  $n/2$  as a lower bound. This, of course, is a worst case lower bound on the length of the encodings of input symbols from  $X$ .

## 7. CONCLUDING REMARKS

We have introduced a mathematical model of proposed molecular switching elements based on soliton propagation along (CH)-chains. Assuming that our model captures the logical aspect of the physico-chemical process well enough, one would assess the computational potential of "soliton valves" with the aid of the purely mathematical results derived for our model.

We have shown that strongly deterministic soliton graphs can simulate precisely the group automata. It is an open problem to characterize the class of groups obtained as transition monoids of strongly deterministic soliton automata. Some of our results seem to indicate that the simulation may be very costly at times. Again, further investigation is required to determine the complexity precisely. In [11], the computational power of strongly deterministic soliton automata is investigated with respect to other notions of simulation.

Although strong determinism is comparatively simple and natural from a mathematical point of view, it seems that general determinism would be more appropriate from a realistic point of view: some useful "soliton valves" have been proposed in [2] which are only deterministic, but not strongly deterministic. The characterization of deterministic soliton automata is more difficult than that of strongly deterministic automata. Some related results will be presented in a separate paper [7].

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